SUPPORTING INFORMATION SECTION

A Mechanistic Understanding of the Degradation of Trace Organic Contaminants by UV/Hydrogen Peroxide, UV/Persulfate and UV/Free Chlorine for Water Reuse

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Submitted to Environmental Sciences: Water Research and Technology

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Text S1 Calculation of photolysis rates

The photolysis rate (r_p) of H_2O_2, $S_2O_8^{2-}$ and HOCl by low-pressure high-output (LPHO) mercury vapor UV lamp (λ=254nm) was calculated based on the following equation:

$$r_p = -2 \times \Phi \times I_0 \times f_{\text{oxidant}} \times f_{\text{solution}} \qquad (1)$$

Φ is the extinction coefficient of the oxidation, *i.e.*, Φ_{H2O2}=0.5 (Baxendale and Wilson, 1957), $\Phi_{persulfate}$=0.7 (Mark et al., 1990), Φ_{HOCl}=0.7 (Watts and Linden, 2007), Φ_{OCl^-}=0.52 (Nowell and Hoigne, 1992). I_o is volume-normalized UV irradiance from the flow-through UV reactor (Scheme S1).

f_{oxidant} is the fraction of incident light absorbed by the oxidant. f_{solution} is the fraction of light absorbed by the total solution, which were calculated as:

$$f_{oxidant} = \frac{\varepsilon_p c_p}{\sum \varepsilon_i c_i} \qquad (2)$$

$$f_{solution} = 1 - 10^{-(\alpha + \sum \varepsilon_i c_i) l} \qquad (3)$$

ε_p is the molar extinction coefficient of the oxidant (M^{-1}•cm^{-1}), c_p is the concentration of the oxidant (M). ε_i and c_i are the molar extinction coefficient and concentration for NOM and a particular contaminant selected. α is the absorption coefficient of the solution at the wavelength of 254 nm and l is the path length of the reactor (cm). The direct photolysis rate for NOM and a particular contaminant is also calculated based on the same equations except $f_{\text{contaminant}}$ is calculated based on the ε_i and c_i of the particular contaminant (refer to Table S3 for the quantum yield and molar extinction coefficient).

The volume-normalized surface irradiance from a flow-through UV reactor (I_o) was calculated as follows:

$$I_0 = \frac{W_{UV} \times S_{UV}}{E_{254nm} \times V \times t} \quad (4)$$

The flow-through UV reactor was based on a configuration widely applied in water reuse facilities (Scheme S1). The hydraulic retention time of the UV reactor (*t*) is 26 second. The energy output of the low-pressure high-output mercury vapor UV lamp (W_{uv}) during the hydraulic retention time of the UV reactor is 1179 mJ (Trojan Technology, London, ON). The UV lamp surface area (S_{uv}) is 1302 cm^2. E is the energy of one mole of photons at the wavelength of 254 nm (4.72×10^8 mJ), V is the volume of the UV reactor (9.8 L). Consequently, I_o was calculated as 1.27×10^{-5} $L^{-1}s^{-1}$.

Text S2 Probe method to determine steady state concentration of radicals

Nitrobenzene, benzoic acid and N,N-dimethylaniline were utilized to probe the steady state concentration of $HO^{\bullet}$, $SO_4^{\bullet-}$, $Cl^{\bullet}$, $Cl_2^{\bullet-}$ and $CO_3^{\bullet-}$. The control experiments showed a negligible direct photo-degradation for all probe compounds. Nitrobenzene exclusively reacts with $HO^{\bullet}$, therefore is the best probe for $HO^{\bullet}$. First, the experimentally observed pseudo first order decay rate of nitrobenzene (k_{obs}) was obtained and $[HO^{\bullet}]_{ss}$ was calculated based on Equation 1.

$$-\ln\left(\frac{[NB]_t}{[NB]_0}\right) = k_{HO-NB}[HO^{\cdot}]_{ss}t \qquad \text{(Eq. 1)}$$

$[NB]_t$ is the concentration of nitrobenzene at time t; $[NB]_0$ is the initial concentration of nitrobenzene; $k_{HO\text{-}NB}$ is the first-order rate constant between $HO^{\bullet}$ and nitrobenzene, *i.e.*, 3.2×10^9 $M^{-1}s^{-1}$, Neta and Dorfman, 1968).

$[CO_3^{\bullet-}]_{ss}$ is calculated based on equation 2 analogously.

$$-\ln\left(\frac{[N,NDMA]_t}{[N,NDMA]_0}\right) = k_{CO3-N,NDMA}[CO_3^{\cdot-}]_{ss}t \qquad \text{(Eq. 2)}$$

$k_{CO3\text{-}NB}$ is the first order rate constant between $CO_3^{\bullet-}$ and N,N-dimethylaniline (1.4×10^9 $M^{-1}s^{-1}$, Lilie et al, 1978).

$[Cl^{\bullet}]_{ss}$ and $[SO_4^{\bullet-}]_{ss}$ were simultaneously calculated using Equationa 3 and 4

$$-\ln\left(\frac{[BA]_t}{[BA]_0}\right) = (k_{HO-BA}[HO^{\cdot}]_{ss} + k_{SO4-BA}[SO_4^{\cdot-}]_{ss} + k_{Cl-BA}[Cl^{\cdot}]_{ss})t \qquad \text{(Eq. 3)}$$

$$-\ln\left(\frac{[1,4D]_t}{[1,4D]_0}\right) = (k_{HO-1,4D}[HO^{\cdot}]_{ss} + k_{SO4-1,4D}[SO_4^{\cdot-}]_{ss} + k_{Cl-1,4D}[Cl^{\cdot}]_{ss})t \qquad \text{(Eq. 4)}$$

$k_{HO\text{-}BA}$=4.3×10^{9} M^{-1}s^{-1}, Wander et al, 1968); $k_{SO4\text{-}BA}$=1.2×10^{9} M^{-1}s^{-1}, Neta et al, 1977); 1.4×10^{9} M^{-1}s^{-1}, $k_{Cl\text{-}BA}$=1.8×10^{10} M^{-1}s^{-1}, Martire et al. 2001).

In the UV/$S_2O_8^{2-}$, the contribution of $Cl_2^{\bullet-}$ to benzoic acid and 1,4-dioxane degradation was minimal because the steady state concentration of $Cl_2^{\bullet-}$ was low and its reactivity with the contaminants was lower than $Cl^{\bullet}$ (Martire et al, 2001). In UV/HOCl system, the steady-state concentration of $Cl_2^{\bullet-}$ could be high enough to make significant contribution to contaminant degradation because the reverse reaction of $ClOH^{\bullet-}$ with Cl^- (Reaction 54 in table S1) produced a significant amount of $Cl_2^{\bullet-}$. Therefore, $[Cl^{\bullet}]_{ss}$ and $[Cl_2^{\bullet-}]_{ss}$ were simultaneously calculated using the following equations:

$$-\ln\left(\frac{[BA]_t}{[BA]_0}\right) = (k_{HO-BA}[HO^{\cdot}]_{ss} + k_{Cl2-BA}[Cl_2^{\cdot-}]_{ss} + k_{Cl-BA}[Cl^{\cdot}]_{ss})t \quad \text{(eq 5)}$$

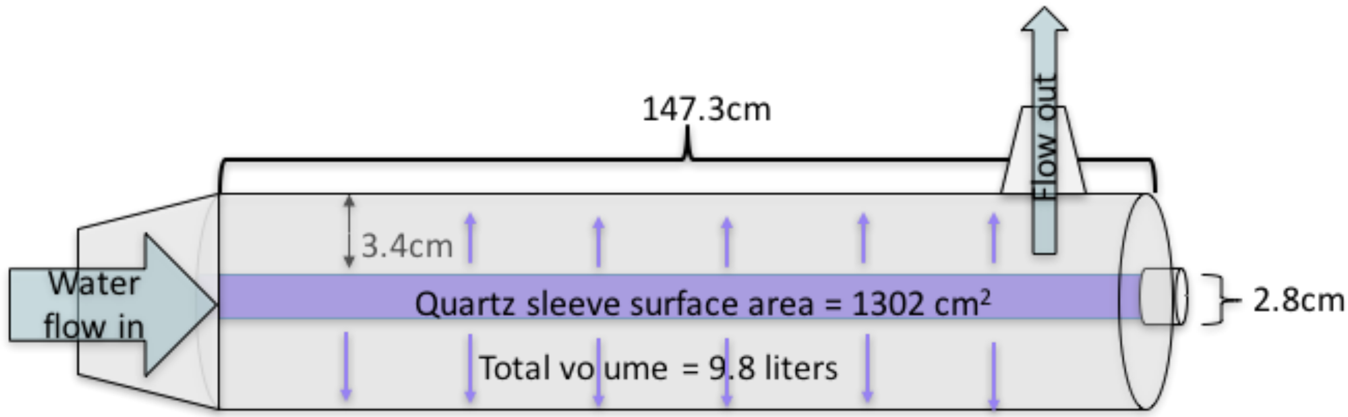
$$-\ln\left(\frac{[1,4D]_t}{[1,4D]_0}\right) = (k_{HO-1,4D}[HO^{\cdot}]_{ss} + k_{Cl2-1,4D}[Cl_2^{\cdot-}]_{ss} + k_{Cl-1,4D}[Cl^{\cdot}]_{ss})t \quad \text{(eq 6)}$$

$k_{Cl2\text{-}BA}$= 1.0×10^{6} - 1.0×10^{8} M^{-1}s^{-1}, $k_{Cl2\text{-}1,4D}$=1.0×10^{6} - 1.0×10^{8} M^{-1}s^{-1} (Text S3).

Text S3 Rate constants of reactions involving radicals

The rate constants for all six compounds were mostly obtained from NIST database (NIST, 2015). When the value was not available, a range of the rate constant was estimated base on existing known values for similar compounds. For example, the reaction mechanism of $Cl^{\bullet}$ and $Br^{\bullet}$ are very similar to $HO^{\bullet}$, and the rates are comparable to the rates of $HO^{\bullet}$ (Grebel et al., 2010, NIST, 2015), thus a ±10% of $HO^{\bullet}$ rate was assigned to $Cl^{\bullet}$ or $Br^{\bullet}$. The estimation also based on the reaction mechanism of the specific radical with different type of molecules. For example, $Cl^{\bullet}$ reacts fast with aromatic compounds and amine containing compounds (10^9-10^{10} $M^{-1}s^{-1}$, NIST, 2015), moderately fast with unsaturated aliphatic compounds (10^8–10^9 $M^{-1}s^{-1}$) and slow with saturated aliphatic compounds including chlorinated or brominated compounds (10^4–10^6 $M^{-1}s^{-1}$). $Br^{\bullet}$ has high reaction rates with aromatic compounds (10^9–10^{10} $M^{-1}s^{-1}$) and low reactivity with aliphatic alcohols (10^4-10^6 $M^{-1}s^{-1}$, NIST, 2015).

A relatively high reactivity also applies to $Cl_2^{\bullet-}$, $ClBr^{\bullet-}$, $Br_2^{\bullet-}$ and $CO_3^{\bullet-}$ (Yang et al., 2014, Fang et al, 2014). Therefore, a ±10% rate was assigned based on known rates for any of the above radicals. With a comparison of available rate constants from the NIST database, $Cl_2^{\bullet-}$ has high reaction rates (10^8 $M^{-1}s^{-1}$) with unsaturated aliphatic compounds than with aromatic (10^6–10^8 $M^{-1}s^{-1}$). Low reactivity with unsaturated carboxylic (10^6 M^{-1} s^{-1}). $CO_3^{\bullet-}$ reacts fast with compounds containing amines (10^8–10^9 $M^{-1}s^{-1}$, NIST, 2015), but low reactivity with aromatic compounds (10^4–10^6 $M^{-1}s^{-1}$). The rates of direct oxidation by HOCl were estimated when the literature values were not available. For example, the oxidation rates for aniline, 17β-estradiol, sulfamethoxazole and carbamazepine by HOCl was estimated based on their known reaction rates with O_3 (Huber et al. 2003). The direct oxidation of 1,4-dioxane by HOCl is negligible based on experimental verification (Figure S1).



Scheme S1 A diagram of the single UV flow-through reactor (Trojan Technologies, London, ON). The kinetics modeling is based on the configuration of this reactor.

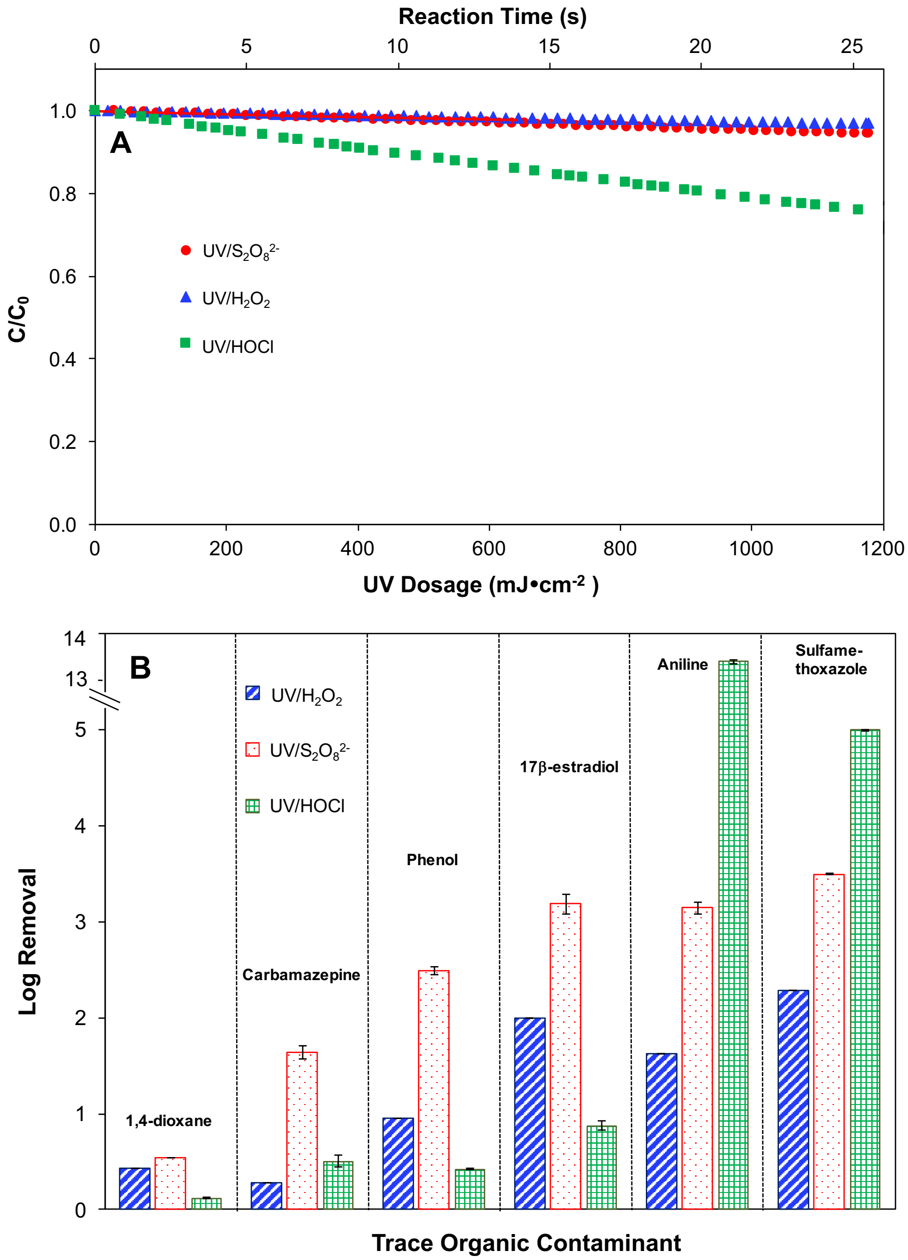


Fig. S1 Comparison of UV/H_2O_2, UV/$S_2O_8^{2-}$ and UV/HOCl treatment based on the kinetic model. (A) Consumption of H_2O_2, $S_2O_8^{2-}$ and HOCl by UV irradiance. (B) Log removal of organic contaminants. [Oxidant]=88 μM, [contaminant]=50 nM, [Cl^-]=80 μM, [inorganic carbon]=200 μM, [Br^-]=0.2 μM, TOC=0.15 mg C/L, pH=8, UV irradiance= 45.3 mW/cm^2, UV dosage=1178 mJ/cm^2 in 26 seconds.

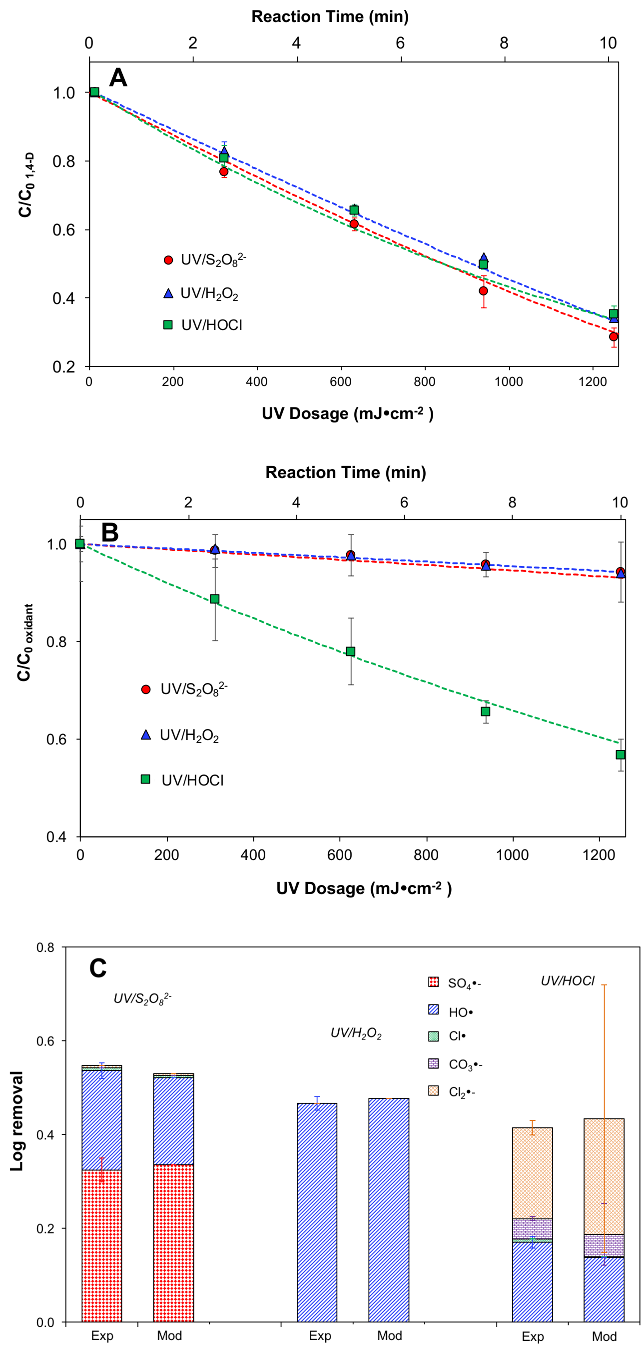


Fig. S2 1,4-dioxane removal byUV/H_2O_2, UV/$S_2O_8^{2-}$ and UV/HOCl. (A) First order decay of 1,4-dioxane. (B) First-order decay of H_2O_2, $S_2O_8^{2-}$ and HOCl by UV irradiance. (C) contribution of radicals to 1,4-dioxane decay. [Oxidant]=2 mM, [1,4-dioxane]=250 μM, [Cl^-]=80 μM, [inorganic carbon]=200 μM, [Br^-]=0.2 μM, TOC=0.15 mg C/L, pH=5.8, UV irradiance= 45.3 mW/cm^2, UV dosage=1178 mJ/cm^2 in 26 seconds. Dash lines are modeled results.

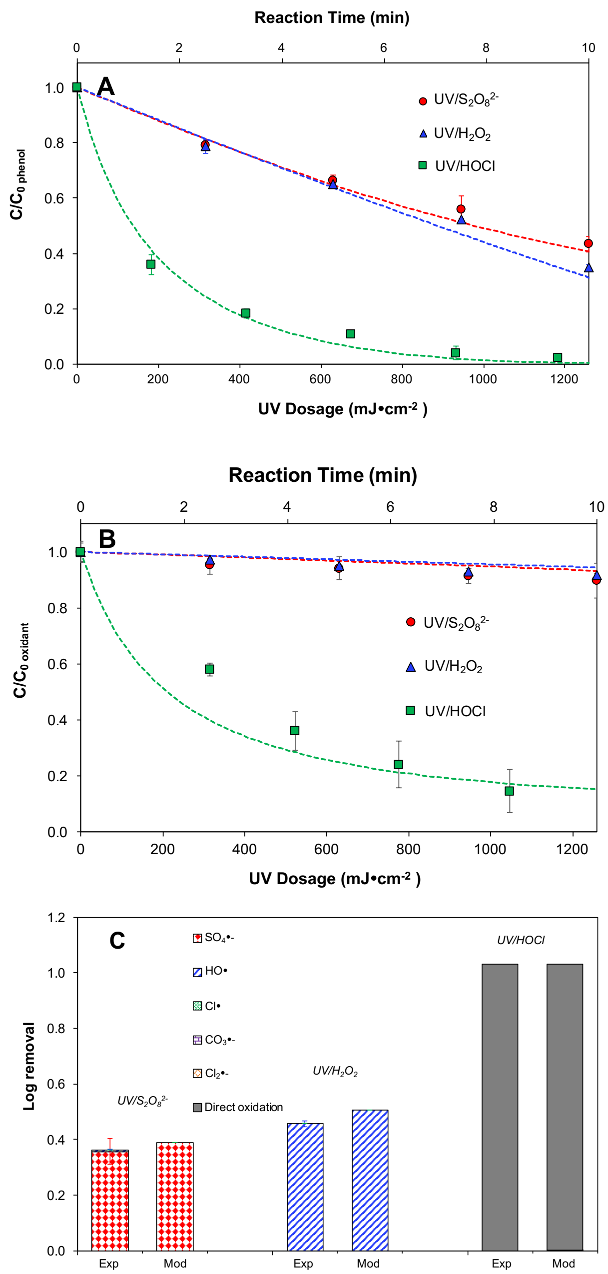


Fig. S3 Phenol removal by UV/H_2O_2, UV/$S_2O_8^{2-}$ and UV/HOCl. (A) First order decay of phenol. (B) First order decay of H_2O_2, $S_2O_8^{2-}$ and HOCl by UV irradiance. (C) Contribution of radicals to phenol decay. [Oxidant]=2 mM, [phenol]=250 μM, [Cl^-]=80 μM, [inorganic carbon]=200 μM, [Br^-]=0.2 μM, TOC=0.15 mg C/L, pH=5.8, UV irradiance= 45.3 mW/cm^2, UV dosage=1178 mJ/cm^2 in 26 seconds. Dash lines are modeled results.

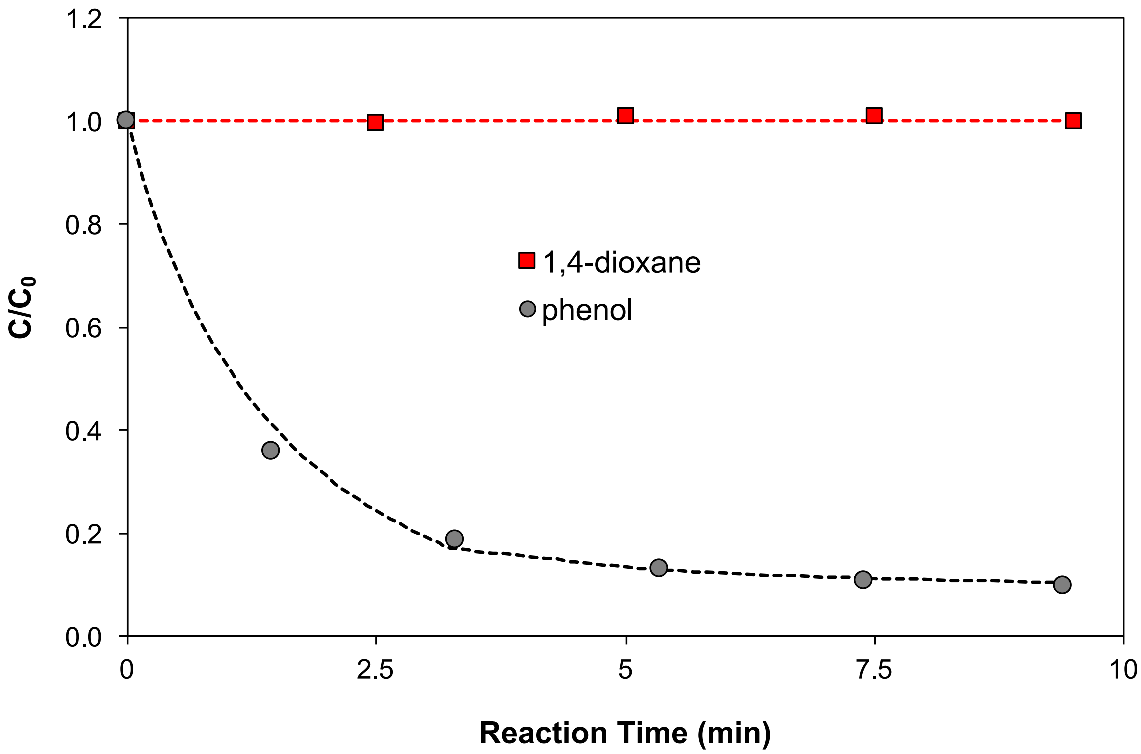


Fig. S4 Direct oxidation of 1,4-dioxane and phenol by HOCl. [Oxidant]=2 mM, [contaminant]=250 μM, [Cl^-]=80 μM, [inorganic carbon]=200 μM, [Br^-]=0.2 μM, TOC=0.15 mg C/L, pH=5.8. Dash lines are modeled results.

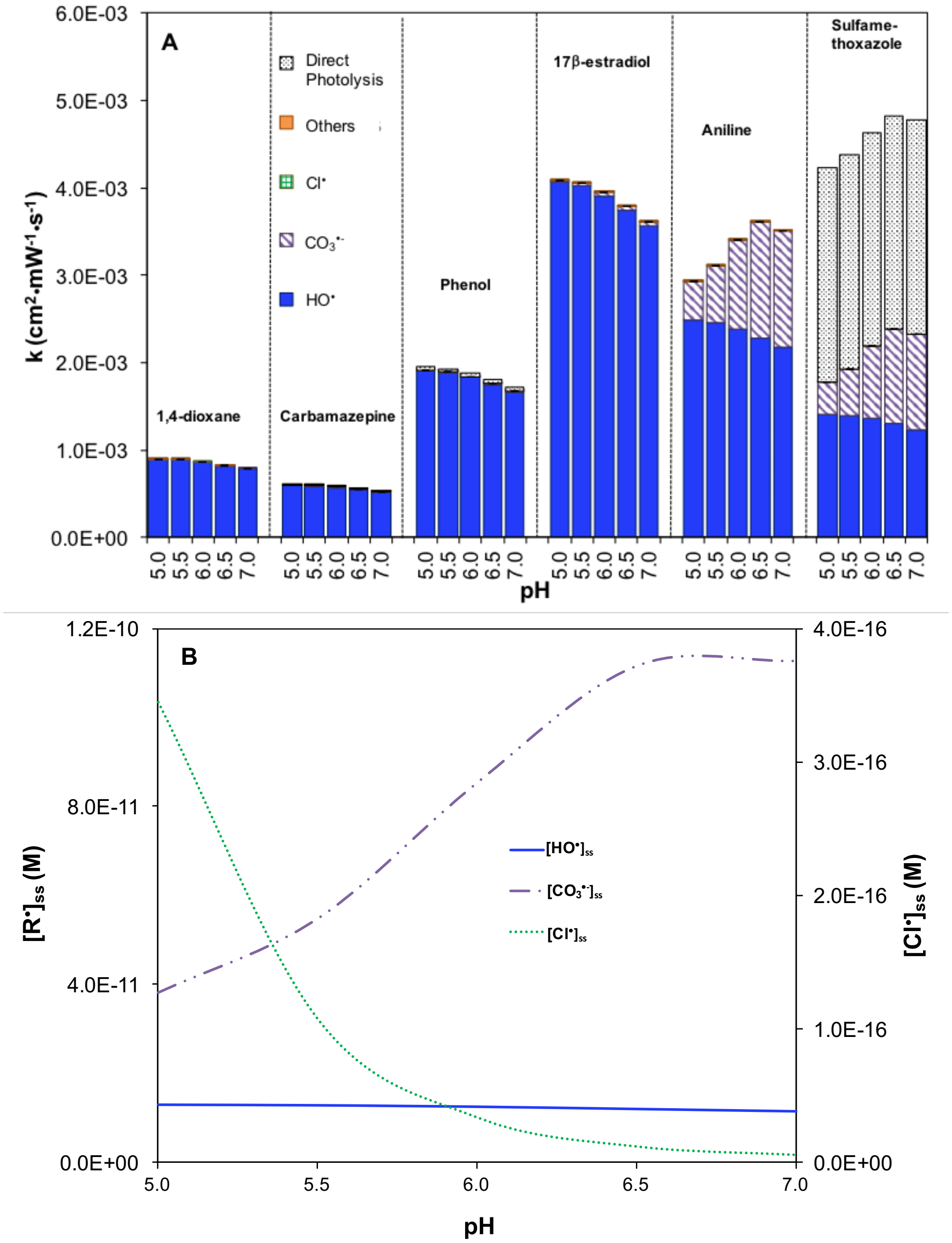
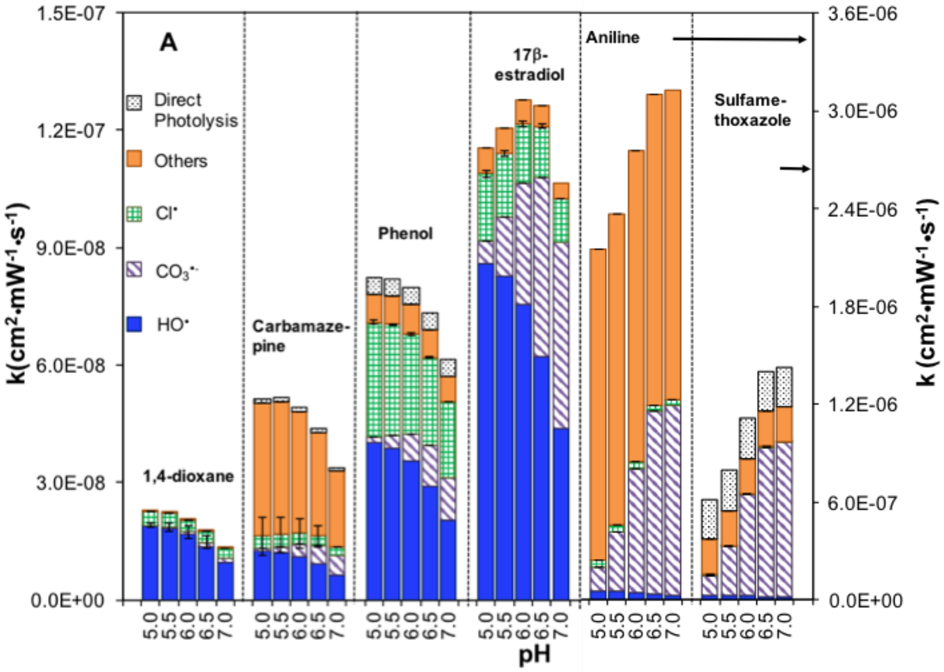


Fig. S5 Effect of pH on the treatment efficiency of UV/H_2O_2 based on the kinetic model. (A) First-order degradation rates of organic contaminants in treatment. (B) Radical distribution. [H_2O_2]=88 µM, [trace organic contaminant]=50 nM, [Cl^-]=0.08 mM, [inorganic carbon]=0.2 mM, [Br^-]=0.2 µM, TOC=0.15 mg C/L, UV irradiance=45 mW/cm^2.



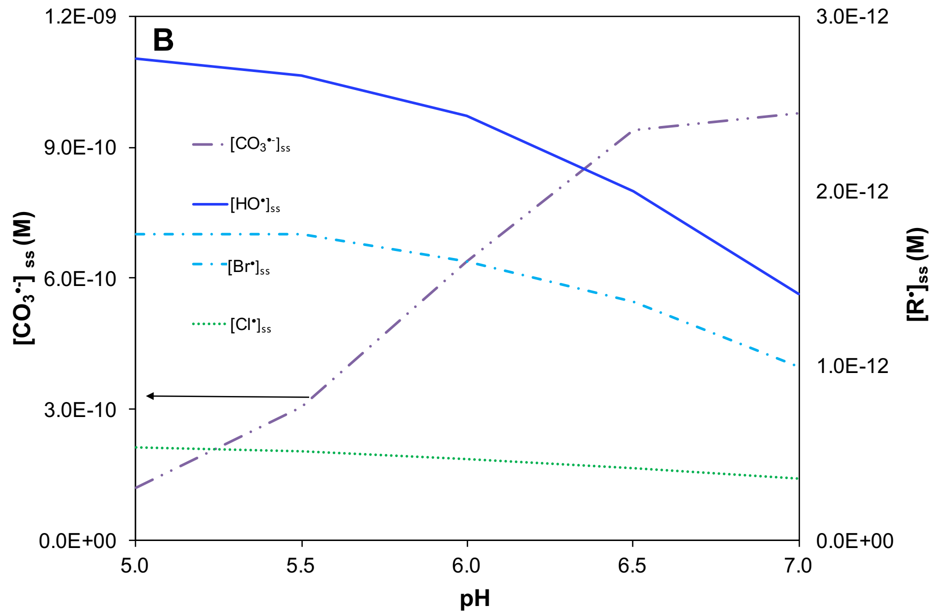


Fig. S6 Effect of pH on the treatment efficiency of UV/HOCl based on the kinetic model. (A) First-order degradation rates of organic contaminants in treatment. (B) Radical distribution. [HOCl]=88 μM, [trace organic contaminant]=50 nM, [Cl^-]=0.08 mM, [inorganic carbon]=0.2 mM, [Br^-]=0.2 μM, TOC=0.15 mg C/L, UV irradiance=45 mW/cm^2.

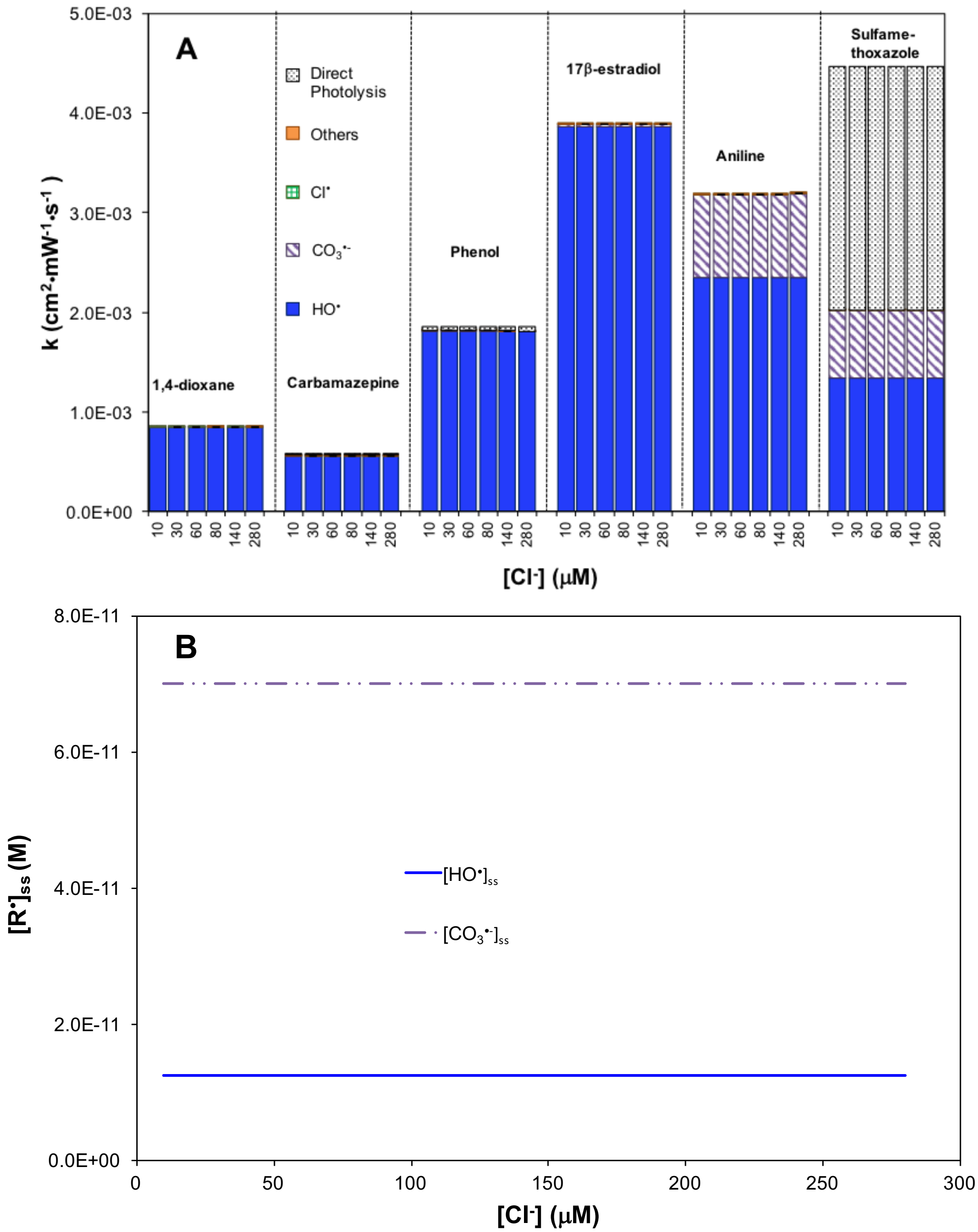


Fig. S7 Effect of chloride on the treatment efficiency of UV/H_2O_2 based on the kinetic model. (A) First-order degradation rates of organic contaminants in treatment. (B) Radical distribution. [H_2O_2]=88 μM, [trace organic contaminant]=50 nM, [inorganic carbon]=0.2 mM, [Br^-]=0.2 μM, pH=5.8, TOC=0.15 mg C/L, UV irradiance=45 mW/cm^2.

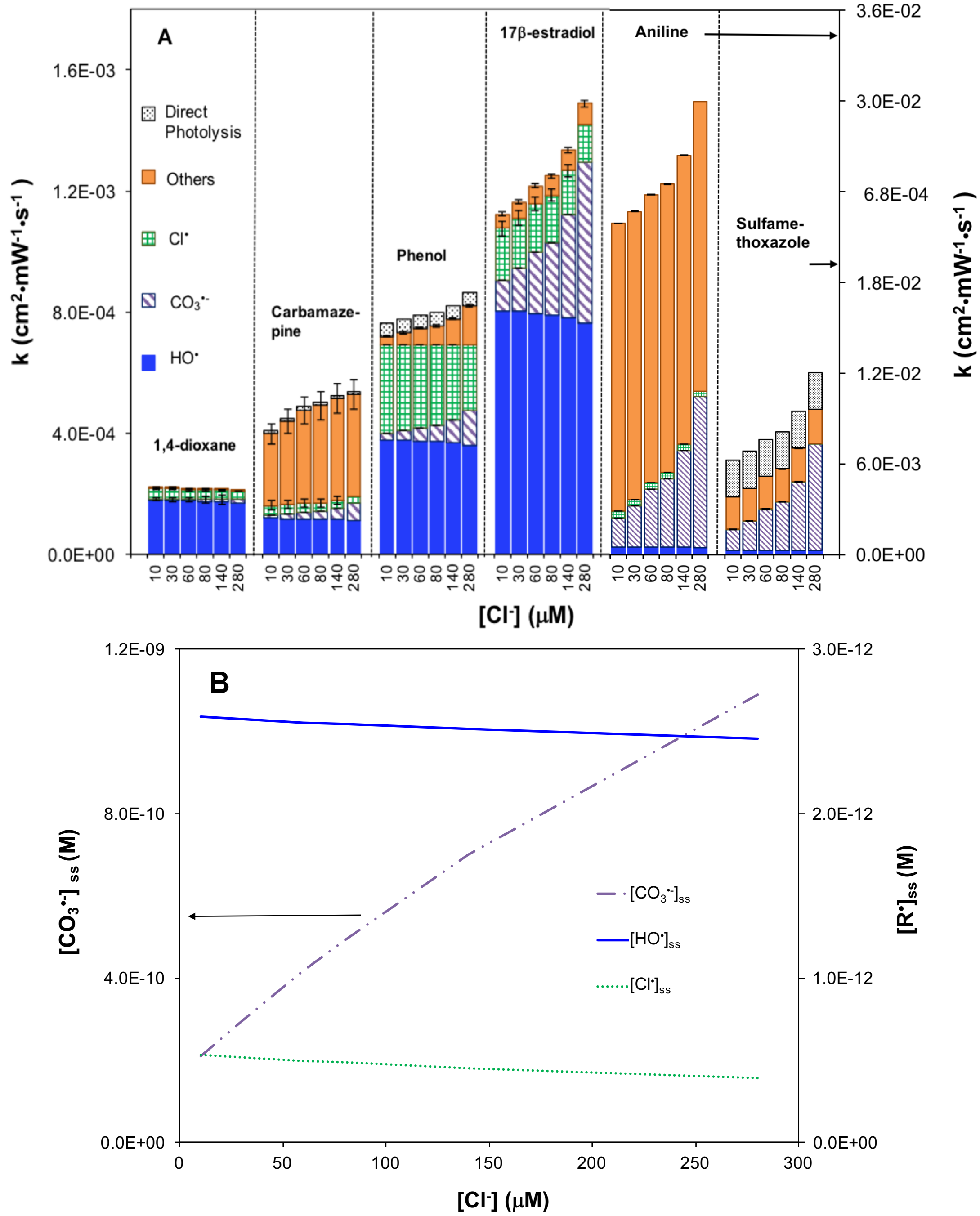


Fig. S8 Effect of chloride on the treatment efficiency of UV/HOCl based on the kinetic model. (A) First-order degradation rates of organic contaminants in treatment. (B) Radical distribution. [HOCl]=88 μM, [trace organic contaminant]=50 nM, [inorganic carbon]=0.2 mM, [Br^-]=0.2 μM, pH=5.8, TOC=0.15 mg C/L, UV irradiance=45 mW/cm^2.

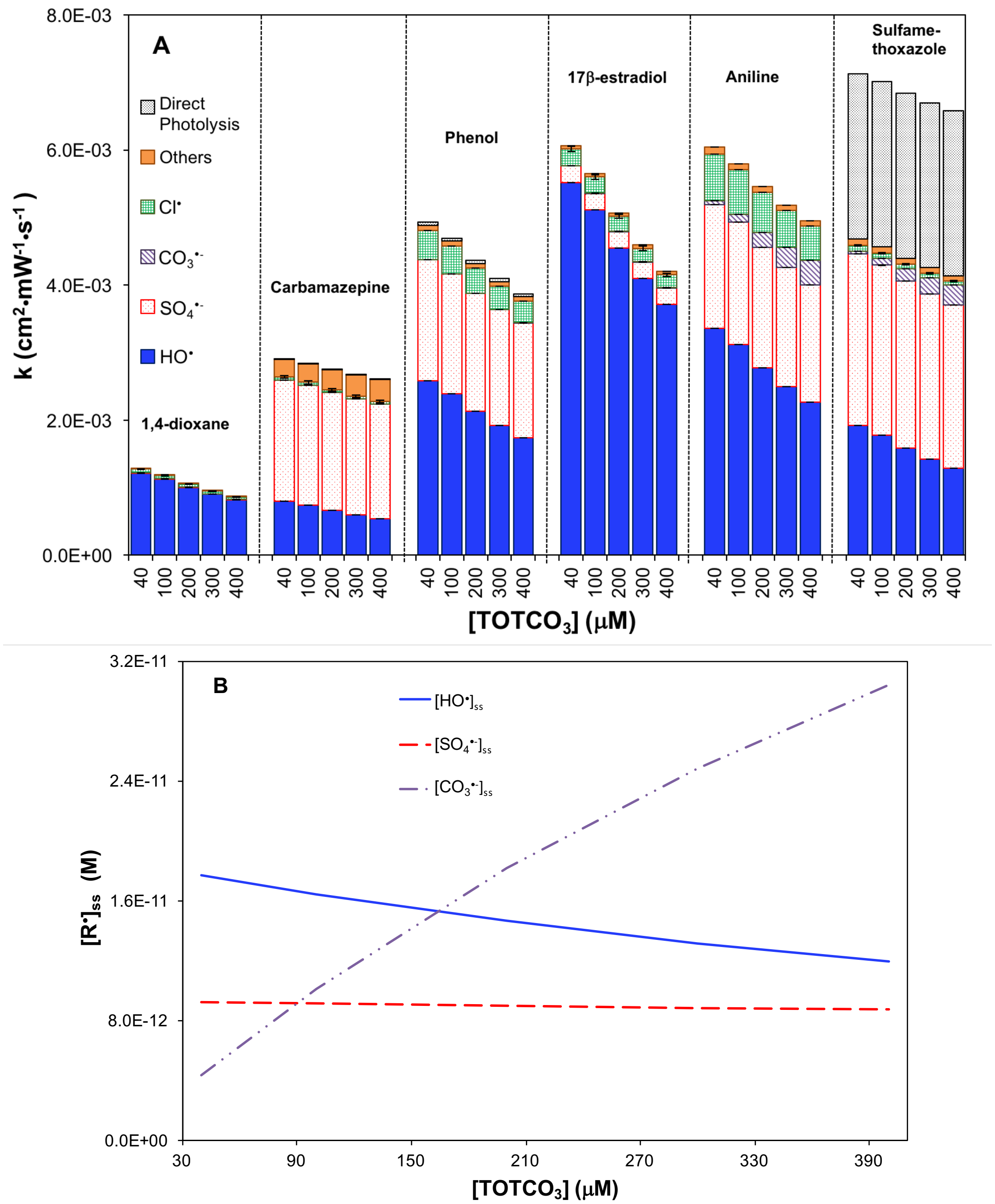


Fig. S9 Effect of inorganic carbon on the treatment efficiency of UV/$S_2O_8^{2-}$ based on the kinetic model. (A) First-order degradation rates of organic contaminants in treatment. (B) Radical distribution. [$S_2O_8^{2-}$]=88 μM, [trace organic contaminant]=50 nM, [Cl^-]=80 μM, [Br^-]=0.2 μM, pH=5.8, TOC=0.15 mg C/L, UV irradiance=45 mW/cm^2.

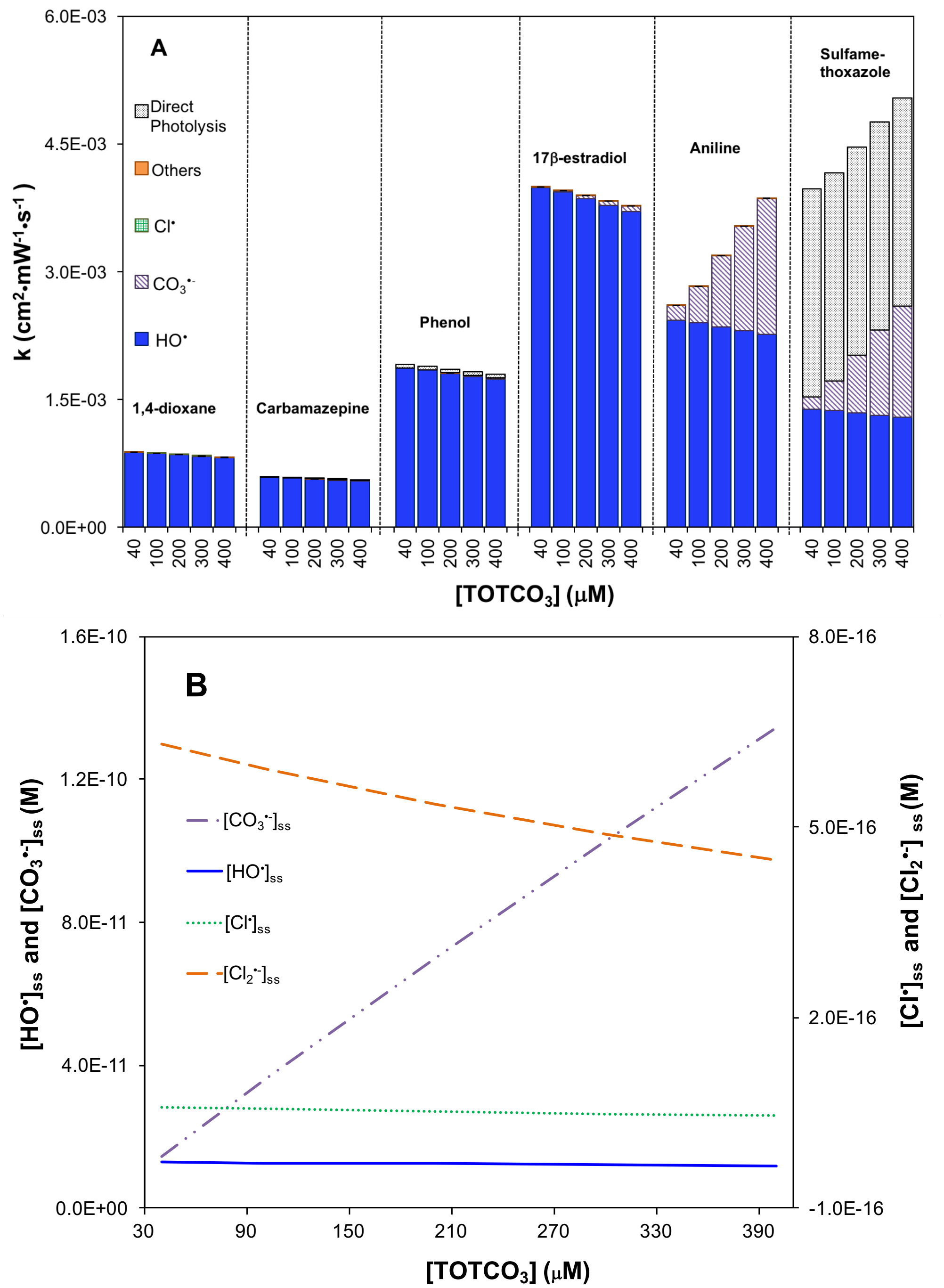


Fig. S10 Effect of inorganic carbon on the treatment efficiency of UV/H_2O_2 based on the kinetic model. (A) First-order degradation rates of organic contaminants in treatment. (B) Radical distribution. [H_2O_2]=88 μM, [trace organic contaminant]=50 nM, [Cl^-]=80 μM, [Br^-]=0.2 μM, pH=5.8, TOC=0.15 mg C/L, UV irradiance=45 mW/cm^2.

Table S1 Rate constants and elemental reactions for kinetics modeling

No.	Reaction	Rate Constant	Reference
1	$H_2O_2 \xrightarrow{h\nu} 2OH^{\cdot}$	1.0×10^{-3} s^{-1}	Calculated
2	$S_2O_8^{2-} \xrightarrow{h\nu} 2SO_4^{\cdot-}$	1.4×10^{-3} s^{-1}	Calculated
3	$HOCl \xrightarrow{h\nu} OH^{\cdot} + Cl^{\cdot}$	3.9×10^{-3} s^{-1}	Calculated
4	$ClO^{-} \xrightarrow{h\nu} Cl^{\cdot} + O^{\cdot-}$	3.2×10^{-3} s^{-1}	Calculated
5	$NOM \xrightarrow{h\nu} OH^{\cdot} + products$	1.8×10^{-10} s^{-1}	Calculated
6	$S_2O_8^{2-} + OH^{\cdot} \rightarrow S_2O_8^{\cdot-}$	1.4×10^{7} $M^{-1}s^{-1}$	Buxton et al., 1990
7	$S_2O_8^{2-} + SO_4^{\cdot-} \rightarrow S_2O_8^{\cdot-} + SO_4^{2-}$	6.6×10^{5} $M^{-1}s^{-1}$	Jiang et al., 1992
8	$S_2O_8^{2-} + Cl^{\cdot} \rightarrow S_2O_8^{\cdot-} + Cl$	8.8×10^{6} $M^{-1}s^{-1}$	Yu et al., 2004
9	$S_2O_8^{2-} + CO_3^{\cdot-} \rightarrow S_2O_8^{\cdot-} + CO_3^{2-}$	3.0×10^{7} $M^{-1}s^{-1}$	Yang et al 2014
10	$S_2O_8^{2-} + SO_5^{\cdot-} \rightarrow S_2O_8^{\cdot-} + SO_5^{2-}$	1.0×10^{5} $M^{-1}s^{-1}$	Assumed
11	$SO_5^{2-} + H^{+} \rightarrow HSO_5^{-}$	5.0×10^{10} $M^{-1}s^{-1}$	Yang et al 2014
12	$SO_5^{2-} + SO_4^{\cdot-} \rightarrow SO_5^{\cdot} + SO_4^{2-}$	1.0×10^{8} $M^{-1}s^{-1}$	Das 2001
13	$HSO_5^{-} \rightarrow H^{+} + SO_5^{2-}$	2.0×10^{1} s^{-1}	Yang et al 2014
14	$HSO_5^{-} + OH^{\cdot} \rightarrow H_2O + SO_5^{\cdot-}$	1.7×10^{7} $M^{-1}s^{-1}$	Maruthamuthu & Neta 1977
15	$SO_4^{\cdot-} + H_2O \rightarrow HSO_4^{2-} + OH^{\cdot}$	6.6×10^{2} s^{-1}	Herrmann et al., 1995
16	$SO_4^{2-} + Cl^{\cdot} \rightarrow SO_4^{\cdot-} + Cl^{-}$	2.5×10^{8} $M^{-1}s^{-1}$	Das 2001
17	$SO_4^{\cdot-} + OH^{-} \rightarrow SO_4^{2-} + OH^{\cdot}$	7.0×10^{7} $M^{-1}s^{-1}$	Peyton 1993
18	$SO_4^{\cdot-} + Cl^{-} \rightarrow SO_4^{2-} + Cl^{\cdot}$	3.0×10^{8} $M^{-1}s^{-1}$	Das 2001
19	$SO_4^{\cdot-} + OH^{\cdot} \rightarrow HSO_5^{-}$	1.0×10^{10} $M^{-1}s^{-1}$	Das 2001
20	$SO_4^{\cdot-} + HSO_5^{-} \rightarrow SO_5^{\cdot-} + SO_4^{2-} + H^{+}$	1.0×10^{6} $M^{-1}s^{-1}$	Das 2001
21	$HSO_4^{-} \rightarrow H^{+} + SO_4^{2-}$	1.2×10^{-2} s^{-1}	Calculated
22	$SO_4^{\cdot-} + SO_4^{\cdot-} \rightarrow S_2O_8^{2-}$	7.0×10^{8} $M^{-1}s^{-1}$	Das 2001
23	$SO_5^{\cdot-} + SO_5^{\cdot-} \rightarrow S_2O_8^{2-} + O_2$	2.2×10^{8} $M^{-1}s^{-1}$	Das 2001
24	$SO_5^{\cdot-} + SO_5^{\cdot-} \rightarrow SO_4^{\cdot-} + SO_4^{\cdot-} + O_2$	2.1×10^{8} $M^{-1}s^{-1}$	Das 2001
25	$SO_5^{\cdot-} + HO_2^{\cdot} \rightarrow O_2 + HSO_5^{-}$	5.0×10^{7} $M^{-1}s^{-1}$	Yermakov et al., 1995
26	$H_2O_2 \rightarrow H^{+} + HO_2^{-}$	1.3×10^{-1} s^{-1}	Yang et al., 2014
27	$H^{+} + HO_2^{-} \rightarrow H_2O_2$	5.0×10^{10} $M^{-1}s^{-1}$	Yang et al., 2014
28	$H_2O_2 + SO_4^{\cdot-} \rightarrow HO_2^{\cdot} + HSO_4^{-}$	1.2×10^{7} $M^{-1}s^{-1}$	Wine et al., 1989
29	$H_2O_2 + SO_4^{\cdot-} \rightarrow HO_2^{\cdot} + SO_4^{2-} + H^{+}$	1.2×10^{7} $M^{-1}s^{-1}$	Maruthamuthu & Neta, 1978
30	$H_2O_2 + O_2^{\cdot-} \rightarrow OH^{\cdot} + OH^{-} + O_2$	1.3×10^{-1} $M^{-1}s^{-1}$	Weinstein & Bielski, 1979
31	$H_2O_2 + O^{\cdot-} \rightarrow O_2^{\cdot-} + H_2O$	4.0×10^{8} $M^{-1}s^{-1}$	Buxton et al., 1988
32	$H_2O \rightarrow H^{+} + OH^{-}$	1.0×10^{-3} s^{-1}	Yang et al., 2014
33	$H^{+} + OH^{-} \rightarrow H_2O$	1.0×10^{11} $M^{-1}s^{-1}$	Yang et al., 2014
34	$H^{+} + O_2^{\cdot-} \rightarrow HO_2^{\cdot}$	5.0×10^{10} $M^{-1}s^{-1}$	Ilan & Rabani, 1976
35	$OH^{\cdot} + H_2O_2 \rightarrow HO_2^{\cdot} + H_2O$	2.7×10^{7} $M^{-1}s^{-1}$	Buxton et al., 1988
36	$OH^{\cdot} + OH^{-} \rightarrow O^{\cdot-} + H_2O$	1.2×10^{10} $M^{-1}s^{-1}$	Buxton et al., 1988
37	$O^{\cdot-} + H_2O \rightarrow OH^{\cdot} + OH^{-}$	1.8×10^{5} s^{-1}	Buxton et al., 1988
38	$O^{\cdot-} + HO_2^{-} \rightarrow O_2^{\cdot-} + OH^{-}$	4.0×10^{8} $M^{-1}s^{-1}$	Buxton et al., 1988
39	$O^{\cdot-} + O_2 \rightarrow O_3^{\cdot-}$	3.6×10^{9} $M^{-1}s^{-1}$	Buxton et al., 1988
40	$O^{\cdot-} + O_2^{\cdot-} + H^{+} \rightarrow OH^{-} + O_2$	6.0×10^{8} $M^{-1}s^{-1}$	Sehested et al., 1982
41	$O_3^{\cdot-} \rightarrow O_2 + O^{\cdot-}$	2.6×10^{3} s^{-1}	Elliot & McCracken 1989
42	$OH^{\cdot} + O^{\cdot-} \rightarrow HO_2^{-}$	1.0×10^{10} $M^{-1}s^{-1}$	Buxton et al., 1988

43	$OH^{\cdot} + HO_2^- \rightarrow HO_2^{\cdot} + OH^-$	7.5×10^9 $M^{-1}s^{-1}$	Christensen et al., 1982
44	$OH^{\cdot} + HO_2^{\cdot} \rightarrow H_2O + O_2$	6.6×10^9 $M^{-1}s^{-1}$	Sehested et al., 1968
45	$OH^{\cdot} + O_2^{\cdot-} \rightarrow OH^- + O_2$	7.0×10^9 $M^{-1}s^{-1}$	Beck, 1969
46	$OH^{\cdot} + OH^{\cdot} \rightarrow H_2O_2$	3.6×10^9 $M^{-1}s^{-1}$	Elliot, 1989
47	$OH^{\cdot} + Cl^- \rightarrow ClOH^{\cdot-}$	4.3×10^9 $M^{-1}s^{-1}$	Jayson et al., 1973
48	$OH^{\cdot} + HSO_4^- \rightarrow H_2O + SO_4^{\cdot-}$	1.7×10^6 $M^{-1}s^{-1}$	Heckel et al., 1966
49	$HO_2^{\cdot} + HO_2^{\cdot} \rightarrow H_2O_2 + O_2$	8.3×10^5 $M^{-1}s^{-1}$	Bielski et al., 1985
50	$HO_2^{\cdot} + H_2O_2 \rightarrow OH^{\cdot} + H_2O + O_2$	3.0×10^0 $M^{-1}s^{-1}$	Koppenol, 1978
51	$HO_2^{\cdot} + O_2^{\cdot-} \rightarrow HO_2^- + O_2$	9.7×10^7 $M^{-1}s^{-1}$	Bielski et al., 1985
52	$HO_2^{\cdot} \rightarrow H^+ + O_2^{\cdot-}$	1.6×10^5 s^{-1}	Bielski et al., 1985
53	$ClOH^{\cdot-} \rightarrow Cl^- + OH^{\cdot}$	6.1×10^9 s^{-1}	Jayson et al., 1973
54	$ClOH^{\cdot-} + Cl^- \rightarrow OH^- + Cl_2^{\cdot-}$	1.0×10^4 $M^{-1}s^{-1}$	Grigorev et al., 1987
55	$ClOH^{\cdot-} + H^+ \rightarrow Cl^{\cdot} + H_2O$	2.1×10^{10} $M^{-1}s^{-1}$	Jayson et al., 1973
56	$HOCl + H_2O_2 \rightarrow HCl + H_2O + O_2$	1.1×10^4 $M^{-1}s^{-1}$	Connick 1947
57	$HOCl + OH^{\cdot} \rightarrow ClO^{\cdot} + H_2O$	2.0×10^9 $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
58	$HOCl + O_2^{\cdot-} \rightarrow Cl^{\cdot} + OH^- + O_2$	7.5×10^6 $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
59	$HOCl + HO_2^{\cdot} \rightarrow Cl^{\cdot} + OH^- + O_2 + H$	7.5×10^6 $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
60	$HOCl + Cl^{\cdot} \rightarrow ClO^{\cdot} + H^+ + Cl^-$	3.0×10^9 $M^{-1}s^{-1}$	Klaning & Thomas, 1985
61	$HOCl + Cl^- \rightarrow Cl_2OH^-$	1.5×10^4 $M^{-1}s^{-1}$	Wang & Margerum, 1994
62	$Cl^{\cdot}+H_2O_2 \rightarrow H^+ + Cl^- + HO_2^{\cdot}$	2.0×10^9 $M^{-1}s^{-1}$	Yu & Barker, 2003
63	$Cl^{\cdot} + H_2O \rightarrow ClOH^{\cdot-} + H^+$	2.5×10^5 s^{-1}	Jayson et al., 1973
64	$Cl^{\cdot} + OH^- \rightarrow ClOH^{\cdot-}$	1.8×10^{10} $M^{-1}s^{-1}$	Klaning & Thomas, 1985
65	$Cl^{\cdot} + Cl^- \rightarrow Cl_2^{\cdot-}$	8.5×10^9 $M^{-1}s^{-1}$	Yu and Barker, 2003
66	$Cl^{\cdot} + Cl_2 \rightarrow Cl_3$	5.3×10^8 $M^{-1}s^{-1}$	Bunce et al, 1985
67	$Cl^{\cdot} + ClO^- \rightarrow ClO^{\cdot} + Cl^-$	8.3×10^9 $M^{-1}s^{-1}$	Klaning & Thomas, 1985
68	$Cl^{\cdot} + Cl^{\cdot} \rightarrow Cl_2$	8.8×10^7 $M^{-1}s^{-1}$	Wu et al., 1980
69	$Cl_2^{\cdot-} + Cl^{\cdot} \rightarrow Cl_2 + Cl^-$	2.1×10^9 $M^{-1}s^{-1}$	Yu & Barker, 2003
70	$Cl_2^{\cdot-} + OH^- \rightarrow Cl^- + ClOH^{\cdot-}$	4.5×10^7 $M^{-1}s^{-1}$	Grigorev et al., 1987
71	$Cl_2^{\cdot-} \rightarrow Cl^{\cdot} + Cl^-$	6.0×10^4 s^{-1}	Yu & Barker, 2003
72	$Cl_2^{\cdot-} + Cl_2^{\cdot-} \rightarrow 2\,Cl^-+Cl_2$	9.0×10^8 $M^{-1}s^{-1}$	Yu & Barker, 2003
73	$Cl_2^{\cdot-} + H_2O \rightarrow Cl^- + HClOH$	1.3×10^3 s^{-1}	Mcelroy, 1990
74	$Cl_2^{\cdot-} + OH^{\cdot} \rightarrow HOCl + Cl^-$	1.0×10^9 $M^{-1}s^{-1}$	Wagner et al., 1986
75	$Cl_2^{\cdot-} + H_2O_2 \rightarrow HO_2^{\cdot} + H^+ + 2\,Cl^-$	1.4×10^5 $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
76	$Cl_2^{\cdot-} + HO_2^{\cdot} \rightarrow O_2 + H^+ + 2\,Cl^-$	3.1×10^9 $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
77	$Cl_2^{\cdot-} + O_2^{\cdot-} \rightarrow O_2 + 2\,Cl^-$	2.0×10^9 $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
78	$HClOH \rightarrow H^+ + ClOH^{\cdot-}$	1.0×10^8 s^{-1}	Mcelroy, 1990
79	$HClOH \rightarrow Cl^{\cdot} + H_2O$	1.0×10^2 s^{-1}	Mcelroy, 1990
80	$HClOH + Cl^- \rightarrow Cl_2^{\cdot-} + H_2O$	5.0×10^9 $M^{-1}s^{-1}$	Mcelroy, 1990
81	$H^+ + Cl^- \rightarrow HCl$	5.0×10^{10} $M^{-1}s^{-1}$	Yang et al 2014
82	$HCl \rightarrow H^+ + Cl^-$	8.6×10^{16} s^{-1}	Yang et al 2014
83	$ClO^- + H_2O_2 \rightarrow Cl^- + H_2O+O_2$	1.7×10^5 $M^{-1}s^{-1}$	Connick 1947
84	$ClO^- + OH^{\cdot} \rightarrow ClO^{\cdot} + OH^-$	8.8×10^9 $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
85	$ClO^- + O_2^{\cdot-} + H_2O \rightarrow Cl^{\cdot} + 2\,OH^- + O_2$	2.0×10^8 $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
86	$Cl_2 + Cl^- \rightarrow Cl_3^{\cdot-}$	2.0×10^4 $M^{-1}s^{-1}$	Ershov, 2004
87	$Cl_2 + O_2^{\cdot-} \rightarrow O_2 + Cl_2^{\cdot-}$	1.0×10^9 $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
88	$Cl_2 + HO_2^{\cdot} \rightarrow H^+ + O_2 + Cl_2^{\cdot-}$	1.0×10^9 $M^{-1}s^{-1}$	Bjergbackke et al., 1981
89	$Cl_2+H_2O \rightarrow HOCl + Cl^- + H^+$	2.2×10^0 s^{-1}	Wang & Margerum, 1994
90	$Cl_2+H_2O_2 \rightarrow 2\,HCl + O_2$	1.3×10^4 $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
91	$Cl_2OH^- \rightarrow HOCl + Cl^-$	5.5×10^9 s^{-1}	Wang & Margerum, 1994

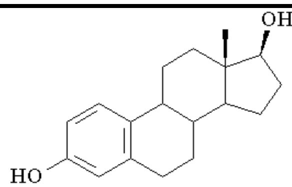
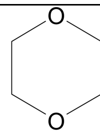
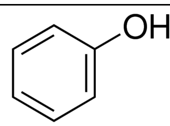
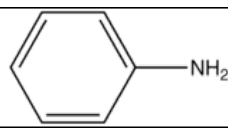
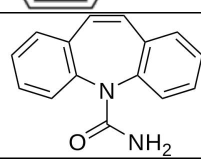
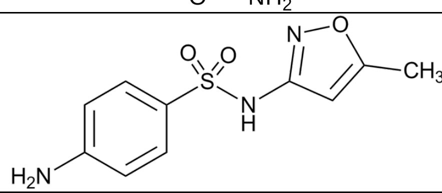
92	$Cl_3^{\cdot-} \rightarrow Cl_2 + Cl^-$	1.1×10^5 s^{-1}	Ershov, 2004
93	$Cl_3^{\cdot-} + HO_2^{\cdot} \rightarrow Cl_2^{\cdot-} + HCl + O_2$	1.0×10^9 M^{-1}s^{-1}	Bjergbackke et al., 1981
94	$Cl_3^{\cdot-} + O_2^{\cdot-} \rightarrow Cl_2^{\cdot-} + Cl^- + O_2$	3.8×10^9 M^{-1}s^{-1}	Matthew & Anastasio, 2006
95	$H_2CO_3 \rightarrow HCO_3^- + H^+$	2.5×10^4 s^{-1}	Yang et al 2014
96	$H_2CO_3 + OH^{\cdot} \rightarrow CO_3^{\cdot-} + H_2O + H^+$	1.0×10^6 M^{-1}s^{-1}	Grebel et al., 2010
97	$HCO_3^- + H^+ \rightarrow H_2CO_3$	5.0×10^{10} M^{-1}s^{-1}	Yang et al 2014
98	$HCO_3^- \rightarrow CO_3^{2-} + H^+$	2.5×10^0 s^{-1}	Matthew & Anastasio, 2006
99	$HCO_3^- + OH^{\cdot} \rightarrow CO_3^{\cdot-} + H_2O$	8.6×10^6 M^{-1}s^{-1}	Buxton et al., 1988
100	$HCO_3^- + Cl^{\cdot} \rightarrow CO_3^{\cdot-} + HCl$	2.2×10^8 M^{-1}s^{-1}	Mertens & von Sonntag, 1995
101	$HCO_3^- + Cl_2^{\cdot-} \rightarrow 2\,Cl^- + H^+ + CO_3^{\cdot-}$	8.0×10^7 M^{-1}s^{-1}	Matthew & Anastasio, 2006
102	$HCO_3^- + SO_4^{\cdot-} \rightarrow CO_3^{\cdot-} + SO_4^{2-} + H^+$	9.1×10^6 M^{-1}s^{-1}	Dogliotti& Hayon, 1967
103	$CO_3^{2-} + H^+ \rightarrow HCO_3^-$	5.0×10^{10} M^{-1}s^{-1}	Matthew & Anastasio, 2006
104	$CO_3^{2-} + OH^{\cdot} \rightarrow CO_3^{\cdot-} + OH^-$	3.9×10^8 M^{-1}s^{-1}	Buxton et al., 1988
105	$CO_3^{2-} + Cl^{\cdot} \rightarrow CO_3^{\cdot-} + Cl^-$	5.0×10^8 M^{-1}s^{-1}	Mertens & von Sonntag, 1995
106	$CO_3^{2-} + Cl_2^{\cdot-} \rightarrow CO_3^{\cdot-} + 2\,Cl^-$	1.6×10^8 M^{-1}s^{-1}	Matthew & Anastasio, 2006
107	$CO_3^{2-} + ClO^{\cdot} \rightarrow CO_3^{\cdot-} + ClO^-$	6.0×10^2 M^{-1}s^{-1}	Huie et al 1991
108	$CO_3^{2-} + SO_4^{\cdot-} \rightarrow CO_3^{\cdot-} + SO_4^{2-}$	2.5×10^6 M^{-1}s^{-1}	Padmaja et al 1993
109	$CO_3^{\cdot-} + H_2O_2 \rightarrow HCO_3^- + HO_2^{\cdot}$	4.3×10^5 M^{-1}s^{-1}	Draganic et al., 1991
110	$CO_3^{\cdot-} + HO_2^- \rightarrow CO_3^{2-} + HO_2^{\cdot}$	3.0×10^7 M^{-1}s^{-1}	Draganic et al., 1991
111	$CO_3^{\cdot-} + HO_2^- \rightarrow HCO_3^- + O_2^{\cdot-}$	3.0×10^7 M^{-1}s^{-1}	Buxton et al., 1990
112	$CO_3^{\cdot-} + OH^{\cdot} \rightarrow product$	3.0×10^9 M^{-1}s^{-1}	Crittenden et al., 1999
113	$CO_3^{\cdot-} + CO_3^{\cdot-} \rightarrow product$	3.0×10^7 M^{-1}s^{-1}	Crittenden et al., 1999
114	$CO_3^{\cdot-} + O_2^{\cdot-} \rightarrow CO_3^{2-} + O_2$	6.0×10^8 M^{-1}s^{-1}	Crittenden et al., 1999
115	$CO_3^{\cdot-} + 2Br^- \rightarrow CO_3^{2-} + Br_2^-$	3.4×10^4 M^{-1}s^{-1}	Huie et al 1991
116	$CO_3^{\cdot-} + ClO^- \rightarrow CO_3^{2-} + ClO^{\cdot}$	5.1×10^5 M^{-1}s^{-1}	Alfassi et al 1988
117	$Br^- + OH^{\cdot} \rightarrow BrOH^{\cdot-}$	1.1×10^{10} M^{-1}s^{-1}	Matthew & Anastasio, 2006
118	$Br^- + SO_4^{\cdot-} \rightarrow Br^{\cdot} + SO_4^{2-}$	3.5×10^9 M^{-1}s^{-1}	Redpath & Willson, 1975
119	$Br^- + H^+ \rightarrow + HBr$	5.0×10^{10} M^{-1}s^{-1}	Yang et al 2014
120	$Br^- + HOCl \rightarrow BrCl + OH^-$	1.3×10^{-1} M^{-1}s^{-1}	Sander et al., 1977
121	$Br^- + Cl_2 \rightarrow BrCl_2^-$	6.0×10^9 M^{-1}s^{-1}	Ershov, 2004
122	$Br^- + ClOH^{\cdot-} \rightarrow BrCl^{\cdot-} + OH^-$	1.0×10^9 M^{-1}s^{-1}	Matthew & Anastasio, 2006
123	$Br^- + Cl^{\cdot} \rightarrow BrCl^{\cdot-}$	1.2×10^{10} M^{-1}s^{-1}	Matthew & Anastasio, 2006
124	$Br^- + Cl_2^{\cdot-} \rightarrow BrCl^{\cdot-} + Cl^-$	4.0×10^9 M^{-1}s^{-1}	Ershov, 2004
125	$Br^- + CO_3^{\cdot-} \rightarrow Br^{\cdot} + CO_3^{2-}$	1.0×10^5 M^{-1}s^{-1}	Mertens & von Sonntag, 1995
126	$Br^- + O^{\cdot-} \rightarrow product$	2.2×10^8 M^{-1}s^{-1}	Rabani & Zehavi, 1971
127	$BrCl_2^- \rightarrow Cl_2 + Br^-$	9.0×10^3 s^{-1}	Ershov, 2004
128	$BrCl_2^- + Br^- \rightarrow Br_2Cl^- + Cl^-$	3.0×10^8 M^{-1}s^{-1}	Ershov, 2004
129	HBr $\rightarrow H^+ + Br^-$	5.0×10^{19} s^{-1}	Yang et al 2014
130	$Br_2 + Br^- \rightarrow Br_3^-$	9.6×10^8 M^{-1}s^{-1}	Matthew & Anastasio, 2006
131	$Br_2 + HO_2^{\cdot} \rightarrow Br_2^{\cdot} + O_2 + H^+$	1.1×10^8 M^{-1}s^{-1}	Matthew & Anastasio, 2006
132	$Br_2 + O_2^{\cdot-} \rightarrow Br_2^{\cdot-} + O_2$	5.6×10^9 M^{-1}s^{-1}	Matthew & Anastasio, 2006
133	$Br_2 + H_2O \rightarrow HOBr + H^+ + Br^-$	9.7×10^1 s^{-1}	Matthew & Anastasio, 2006
134	$Br_2 + H_2O_2 \rightarrow HBr + O_2$	1.3×10^3 M^{-1}s^{-1}	Wagner & Strehlow, 1987
135	$Br_2 + Cl^- \rightarrow Br_2\,Cl^-$	5.0×10^4 M^{-1}s^{-1}	Matthew & Anastasio, 2006
136	$Br_2Cl^- \rightarrow +Br_2 + Cl^-$	3.8×10^4 s^{-1}	Matthew & Anastasio, 2006
137	$Br_2Cl^- + Cl^- \rightarrow BrCl_2^- + Br^-$	1.0×10^5 M^{-1}s^{-1}	Matthew& Anastasio, 2006
138	$Br_3^- \rightarrow Br_2$	5.5×10^7 s^{-1}	Matthew & Anastasio, 2006
140	$Br_3^- + HO_2^{\cdot} \rightarrow Br_2^{\cdot-} + HBr + O_2$	1.0×10^7 M^{-1}s^{-1}	Matthew & Anastasio, 2006
141	$Br_3^- + O_2^{\cdot-} \rightarrow Br_2^{\cdot-} + Br^- + O_2$	3.8×10^9 M^{-1}s^{-1}	Matthew & Anastasio, 2006

142	$OBr^- + H^+ \rightarrow HOBr$	5.0×10^{10} M^{-1}s^{-1}	Yang et al 2014
143	$OBr^- + H_2O_2 \rightarrow Br^- + H_2O + O_2$	1.2×10^{6} M^{-1}s^{-1}	von Gunten & Oliveras, 1997
144	$OBr^- + OH^{\cdot} \rightarrow BrO^{\cdot} + OH^-$	4.5×10^{9} M^{-1}s^{-1}	Matthew & Anastasio, 2006
145	$OBr^- + O_2^{\cdot-} + H_2O \rightarrow Br^{\cdot} + 2\,OH^- + O_2$	2.0×10^{8} M^{-1}s^{-1}	Matthew & Anastasio, 2006
146	$OBr^- + CO_3^{\cdot-} \rightarrow CO_3^{2-} + BrO^{\cdot}$	4.3×10^{7} M^{-1}s^{-1}	Buxton & Dainton 1968
147	$OBr^- + O^{\cdot-} + H^+ \rightarrow OH^- + BrO^{\cdot}$	2.9×10^{9} M^{-1}s^{-1}	Czapski & Treinin, 1969
148	$HOBr \rightarrow H^+ + OBr^-$	7.9×10^{1} s^{-1}	Yang et al 2014
149	$HOBr + Br^- + H^+ \rightarrow Br_2 + H_2O$	5.0×10^{9} M^{-1}s^{-1}	Eigen & Kustin, 1962
150	$HOBr + HO_2^- \rightarrow Br^- + H_2O + O_2$	7.6×10^{8} M^{-1}s^{-1}	von Gunten & Oliveras, 1997
151	$HOBr + H_2O_2 \rightarrow HBr + H_2O + O_2$	1.5×10^{4} M^{-1}s^{-1}	von Gunten & Oliveras, 1997
152	$HOBr + OH^{\cdot-} \rightarrow BrO^{\cdot} + H_2O$	2.0×10^{9} M^{-1}s^{-1}	Matthew & Anastasio, 2006
153	$HOBr + O_2^{\cdot-} \rightarrow BrOH^{\cdot-} + O_2$	3.5×10^{9} M^{-1}s^{-1}	von Gunten & Oliveras, 1997
154	$HOBr + HO_2^{\cdot} \rightarrow BrOH^{\cdot-} + H^+ + O_2$	3.5×10^{9} M^{-1}s^{-1}	Matthew & Anastasio, 2006
155	$HOBr + Cl^- \rightarrow BrCl + OH^-$	5.6×10^{2} M^{-1}s^{-1}	Sander et al., 1977
156	$Br^{\cdot} + H_2O \rightarrow BrOH^{\cdot-} + H^+$	1.4×10^{0} s^{-1}	Klaning & Wolff, 1985
157	$Br^{\cdot} + OH^- \rightarrow BrOH^{\cdot-}$	1.1×10^{10} M^{-1}s^{-1}	Zehavi & Rabani, 1972
158	$Br^{\cdot} + Br^- \rightarrow Br_2^{\cdot-}$	1.2×10^{10} M^{-1}s^{-1}	Matthew & Anastasio, 2006
159	$Br^{\cdot} + Br^{\cdot} \rightarrow Br_2$	1.0×10^{9} M^{-1}s^{-1}	Matthew & Anastasio, 2006
160	$Br^{\cdot} + OBr^- \rightarrow Br^- + BrO^{\cdot}$	4.1×10^{9} M^{-1}s^{-1}	Klaning & Wolff 1985
161	$Br^{\cdot} + H_2O_2 \rightarrow HO_2^{\cdot} + Br^- + H^+$	4.0×10^{9} M^{-1}s^{-1}	Matthew & Anastasio, 2006
162	$Br^{\cdot} + HO_2^{\cdot} \rightarrow H^+ + O_2 + Br^-$	1.6×10^{8} M^{-1}s^{-1}	Matthew & Anastasio, 2006
163	$Br^{\cdot} + CO_3^{2-} \rightarrow Br^- + CO_3^{\cdot-}$	2.0×10^{6} M^{-1}s^{-1}	Matthew & Anastasio, 2006
164	$Br^{\cdot} + HCO_3^- \rightarrow Br^- + CO_3^{\cdot-}$	1.0×10^{6} M^{-1}s^{-1}	Matthew & Anastasio, 2006
165	$Br^{\cdot} + Cl^- \rightarrow BrCl^{\cdot-}$	1.0×10^{8} M^{-1}s^{-1}	Matthew & Anastasio, 2006
166	$Br_2^{\cdot-} + H_2O_2 \rightarrow HO_2^{\cdot} + 2Br^- + H^+$	5.0×10^{2} M^{-1}s^{-1}	Matthew & Anastasio, 2006
167	$Br_2^{\cdot-} \rightarrow Br^{\cdot} + Br^-$	1.9×10^{4} s^{-1}	Matthew & Anastasio, 2006
168	$Br_2^{\cdot-} + Br_2^{\cdot-} \rightarrow Br_2 + 2Br^-$	1.9×10^{9} M^{-1}s^{-1}	Matthew & Anastasio, 2006
169	$Br_2^{\cdot-} + Br^{\cdot} \rightarrow Br_2 + Br^-$	2.0×10^{9} M^{-1}s^{-1}	Matthew & Anastasio, 2006
170	$Br_2^{\cdot-} + HO_2^{\cdot} \rightarrow O_2 + 2Br^- + H^+$	1.0×10^{8} M^{-1}s^{-1}	Wagner & Strehlow, 1987
171	$Br_2^{\cdot-} + HO_2^{\cdot} \rightarrow HO_2^{\cdot}$	4.4×10^{9} M^{-1}s^{-1}	Matthew & Anastasio, 2006
172	$Br_2^{\cdot-} + O_2^{\cdot-} \rightarrow O_2 + 2Br^-$	1.7×10^{8} M^{-1}s^{-1}	Wagner & Strehlow, 1987
173	$Br_2^{\cdot-} + OBr^- \rightarrow BrO^{\cdot} + 2Br^-$	6.2×10^{7} M^{-1}s^{-1}	Matthew & Anastasio, 2006
174	$Br_2^{\cdot-} + OH^{\cdot} \rightarrow HOBr + Br^-$	1.0×10^{9} M^{-1}s^{-1}	Wagner & Strehlow, 1987
175	$Br_2^{\cdot-} + OH^- \rightarrow BrOH^{\cdot-} + Br^-$	2.7×10^{6} M^{-1}s^{-1}	Manou et al., 1977
176	$Br_2^{\cdot-} + CO_3^{2-} \rightarrow 2Br^- + CO_3^{\cdot-}$	1.1×10^{5} M^{-1}s^{-1}	Matthew & Anastasio, 2006
177	$Br_2^{\cdot-} + HCO_3^- \rightarrow 2Br^- + CO_3^{\cdot-} + H^+$	8.0×10^{4} M^{-1}s^{-1}	Matthew & Anastasio, 2006
178	$Br_2^{\cdot-} + Cl^- \rightarrow BrCl^{\cdot-} + Br^-$	4.3×10^{6} M^{-1}s^{-1}	Ershov, 2004
179	$Br_2^{\cdot-} + Cl_2^{\cdot-} \rightarrow Br_2 + 2\,Cl^-$	4.0×10^{9} M^{-1}s^{-1}	Matthew & Anastasio, 2006
180	$BrOH^{\cdot-} \rightarrow OH^{\cdot} + Br^-$	3.3×10^{7} s^{-1}	Zehavi and Rabani, 1972
181	$BrOH^{\cdot-} \rightarrow Br^{\cdot} + OH^-$	4.2×10^{6} s^{-1}	Zehavi and Rabani, 1972
182	$BrOH^{\cdot-} + H^+ \rightarrow Br^{\cdot} + H_2O$	4.4×10^{10} M^{-1}s^{-1}	Zehavi and Rabani, 1972
183	$BrOH^{\cdot-} + Br^- \rightarrow Br_2^{\cdot-} + OH^-$	1.9×10^{8} M^{-1}s^{-1}	Zehavi and Rabani, 1972
184	$BrOH^{\cdot-} + Cl^- \rightarrow BrCl^{\cdot-} + OH^-$	1.9×10^{8} M^{-1}s^{-1}	Matthew & Anastasio, 2006
185	$Br_2OH^- + H^+ \rightarrow Br_2 + H_2O$	2.0×10^{10} M^{-1}s^{-1}	Eigen and Kustin, 1962
186	$Br_2OH^- \rightarrow HOBr + Br^-$	5.0×10^{9} s^{-1}	Eigen and Kustin, 1962
187	$BrCl + H_2O \rightarrow HOBr + Cl^- + H^+$	1.0×10^{5} s^{-1}	Matthew & Anastasio, 2006
188	$BrCl + H_2O_2 \rightarrow HBr + HCl + O_2$	1.3×10^{4} M^{-1}s^{-1}	Matthew & Anastasio, 2006
189	$BrCl + O_2^{\cdot-} \rightarrow BrCl^{\cdot-} + O_2$	4.0×10^{9} M^{-1}s^{-1}	Matthew & Anastasio, 2006
190	$BrCl + HO_2^{\cdot} \rightarrow BrCl^{\cdot-} + O_2 + H^+$	5.0×10^{8} M^{-1}s^{-1}	Matthew & Anastasio, 2006

191	$BrCl + Cl^{-} \rightarrow BrCl_2^{-}$	1.0×10^{6} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
192	$BrCl + Br^{-} \rightarrow Br_2Cl^{-}$	3.0×10^{8} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
193	$BrCl^{\cdot -} + OH^{\cdot} \rightarrow BrCl + OH^{-}$	1.0×10^{9} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
194	$BrCl^{\cdot -} + HO_2^{\cdot} \rightarrow Br^{-} + Cl^{-} + O_2 + H^{+}$	1.0×10^{9} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
195	$BrCl^{\cdot -} + O_2^{\cdot -} \rightarrow Br^{-} + Cl^{-} + O_2$	6.0×10^{8} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
196	$BrCl^{\cdot -} + H_2O_2 \rightarrow Br^{-} + HCl + HO_2$	5.0×10^{3} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
197	$BrCl^{\cdot -} + OH^{-} \rightarrow Br^{-} + ClOH^{-}$	3.0×10^{6} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
198	$BrCl^{\cdot -} + OH^{-} \rightarrow BrOH^{\cdot -} + Cl^{-}$	2.0×10^{7} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
199	$BrCl^{\cdot -} + HCO_3^{-} \rightarrow Br^{-} + HCl + CO_3^{\cdot -}$	3.0×10^{6} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
200	$BrCl^{\cdot -} + CO_3^{2-} \rightarrow Br^{-} + Cl^{-} + CO_3^{\cdot -}$	6.0×10^{6} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
201	$BrCl^{\cdot -} + BrCl^{\cdot -} \rightarrow Br^{-} + Cl^{-} + BrCl$	4.7×10^{9} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
202	$BrCl^{\cdot -} + Cl_2^{\cdot -} \rightarrow 2Cl^{-} + BrCl$	2.0×10^{9} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
203	$BrCl^{\cdot -} + Br_2^{\cdot -} \rightarrow Br_2 + Cl^{-} + Br^{-}$	4.0×10^{9} $M^{-1}s^{-1}$	Matthew & Anastasio, 2006
204	$BrCl^{\cdot -} \rightarrow Cl^{\cdot} + Br^{-}$	2.0×10^{3} s^{-1}	Donati 2002
205	$BrCl^{\cdot -} \rightarrow Cl^{-} + Br^{\cdot}$	6.1×10^{4} s^{-1}	Donati 2002
206	$BrCl^{\cdot -} + Br^{-} \rightarrow Br_2^{\cdot -} + Cl^{-}$	8.0×10^{9} $M^{-1}s^{-1}$	Ershov, 2004
207	$BrCl^{\cdot -} + Cl^{-} \rightarrow Cl_2^{\cdot -} + Br^{-}$	1.1×10^{2} $M^{-1}s^{-1}$	Ershov, 2004
208	$Br_2Cl^{-} \rightarrow BrCl + Br^{-}$	1.7×10^{4} s^{-1}	Matthew & Anastasio, 2006
209	$Br_2Cl^{-} \rightarrow BrCl + Cl^{-}$	1.7×10^{5} s^{-1}	Ershov, 2004
210	$NOM + OH^{\cdot} \rightarrow product$	7.2×10^{4} $(mg/L)^{-1}s^{-1}$	Jasper and Sedlak, 2013
211	$NOM + SO_4^{\cdot -} \rightarrow product$	2.5×10^{4} $(mg/L)^{-1}s^{-1}$	Lutze et al 2015
212	$NOM + Cl^{\cdot} \rightarrow product$	1.3×10^{4} $(mg/L)^{-1}s^{-1}$	Fang et al 2014
213	$NOM + Cl_2^{\cdot -} \rightarrow product$	1.0×10^{2} $(mg/L)^{-1}s^{-1}$	Assumed, refer to text S3
214	$NOM + CO_3^{\cdot -} \rightarrow product$	3.7×10^{2} $(mg/L)^{-1}s^{-1}$	Jasper and Sedlak 2013
215	$NOM + Br^{\cdot} \rightarrow product$	1.0×10^{4} $(mg/L)^{-1}s^{-1}$	*
216	$NOM + Br_2^{\cdot -} \rightarrow product$	1.0×10^{2} $(mg/L)^{-1}s^{-1}$	*
217	$NOM + BrCl^{\cdot -} \rightarrow product$	1.0×10^{2} $(mg/L)^{-1}s^{-1}$	*
218	$HOCl + Aniline \rightarrow product$	9.0×10^{3} $M^{-1}s^{-1}$	*
219	$HOCl + 17\beta - estrodiol \rightarrow product$	2.5×10^{2} $M^{-1}s^{-1}$	*
220	$HOCl + sulfamethoxazoel \rightarrow product$	1.0×10^{2} $M^{-1}s^{-1}$	*
221	$HOCl + carbamezepine \rightarrow product$	1.0×10^{2} $M^{-1}s^{-1}$	*

* Rate constants are estimated (detail in Text S3)

Table S2 Compound structure and their quantum yield, extinction coefficient and direct photolysis rate

Compound Name	Structure	Direct Photolysis Rate (s^{-1})	Reference
17b-estradiol		Negligible	Mendez et al., 2010
1,4-dioxane		Negligible	Stefan and Bolton, 1998
Phenol		2.1×10^{-4}*	Prahl, 2012
Aniline		Negligible	Tang et al., 2010
Carbamazepine		4.6×10^{-4}*	Pereira et al.,
Sulfamethoxazole		1.1×10^{-4}*	Zhang et al., 2015
Natural Organic Matter (NOM)		1.8×10^{-10}*	Jasper et al., 2013 Doll & Frimmel, 2003

* Calculated based on Equations 1-3 in the main text. $\Phi_{NOM}=3.7 \times 10^{-5}$ mole/Einstein, $\varepsilon_{NOM}=5.0\times10^{-2}$ L $mg^{-1}cm^{-1}$, $\Phi_{phenol}=4.15\times10^{-2}$ mole/Einstein, $\varepsilon_{\lambda phenol}=7.50\times10^{2}$ $M^{-1}cm^{-1}$, $\Phi_{carba}=6.0\times10^{-4}$ mole/Einstein, $\varepsilon_{\lambda carba}=8.0\times10^{3}$ $M^{-1}cm^{-1}$ (2007), $\Phi_{smx}= 7.2\times10^{-2}$ mole/Einstein, $\varepsilon_{\lambda smx}=1.6\times10^{4}$ $M^{-1}cm^{-1}$.

Table S3 Rate constants of reactions between selected organic contaminants and radicals

Contaminant	$HO^{\bullet}$ ($M^{-1}s^{-1}$)	$SO_4^{\bullet-}$ (M^{-1} s^{-1})	$Cl^{\bullet}$ (M^{-1} s^{-1})	$Cl_2^{\bullet-}$ (M^{-1} s^{-1})	$ClOH^{\bullet-}$ (M^{-1} s^{-1})
17β-estradiol	1.4×10^{10} Rosenfeldt and Linden, 2004	1.2×10^{9} Rickman et al., 2010	$1.3–1.6\times10^{10}$*	$2.0–2.4\times10^{7}$ *	$2.0–2.4\times10^{7}$ *
Phenol	6.6×10^{9} Lindsey and Tarr, 2000	8.8×10^{9} Lindsey and Tarr, 2000	2.5×10^{10} Alfassi et al, 1989	3.2×10^{8} Alfassi et al, 1990	$5.0–6.0\times10^{6}$ *
Aniline	8.6×10^{9} Qin et al., 1985	9.0×10^{9} Ahmed et al., 2012	4.0×10^{10} Alfassi et al., 1989	$3.4–4.1\times10^{8}$	$3.4–4.1\times10^{8}$
Sulfamethoxazole	4.9×10^{9} Boreen et al., 2004/2005	1.3×10^{10} Ahmed et al. 2012	$4.4\sim5.4\times10^{9}$*	$4.0–4.8\times10^{8}$ *	$4.0–4.8\times10^{8}$ *
1,4-dioxane	3.1×10^{9} Eibenberger, 1980	4.1×10^{7} Huie et al., 1991	$2.8–3.4\times10^{9}$*	$1.0\times10^{5-6}$*	$1.0\times10^{5-6}$*
Carbamazepine	2.1×10^{9} Vogna et al., 2004	8.8×10^{9} Huber et al., 2003	$1.8–3.7\times10^{9}$*	$2.1–2.5\times10^{6}$ *	$2.1–2.5\times10^{6}$ *

Table S3 (Continued from the previous page)

Contaminant	**$CO_3^{\cdot-}$ (M^{-1} s^{-1})**	**$Br^{\cdot}$ (M^{-1} s^{-1})**	**$Br_2^{\cdot-}$ (M^{-1} s^{-1})**	**$ClBr^{\cdot-}$ (M^{-1} s^{-1})**
17β-estradiol	2.2×10^{7} Jasper and Sedlak, 2013	$1.3–1.6\times10^{9}$*	$2.0–2.4\times10^{7}$ *	$2.0–2.4\times10^{7}$ *
Phenol	4.9×10^{6} Chen et al., 1975	$5.9–7.3\times10^{8}$ *	6.0×10^{6} Simic et al., 1974	$5.0–6.0\times10^{6}$ *
Aniline	5.4×10^{8} Chen et al., 1975	$7.7–9.5\times10^{8}$ *	2.1×10^{8} Qin et al., 1985	$3.4–4.1\times10^{8}$
Sulfamethoxazole	4.4×10^{8} Jasper and Sedlak, 2013	$4.4–5.4\times10^{8}$*	$4.0–4.8\times10^{8}$ *	$4.0–4.8\times10^{8}$ *
1,4-dioxane	$1.0\times10^{2\text{-}6}$* Chen et al., 1975	1.2×10^{6} Scaiano et al., 1993	$1.0\times10^{5\text{-}6}$*	$1.0\times10^{5\text{-}6}$*
Carbamazepine	2.3×10^{6} Jasper and Sedlak, 2013	$7.9–9.7\times10^{9}$*	$2.1–2.5\times10^{6}$ *	$2.1–2.5\times10^{6}$ *

* Rates constants are estimated base on the known reactivity of radicals with other similar compounds (details in Text S3)

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